

Upgrades to the R-Matrix Code SAMMY

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Abstract. The analysis code SAMMY is widely used for parameterization and understanding of neutron- and charged-particle-induced cross section data. This report describes advances made in the development of the code: An overview of the main features of SAMMY is presented, with emphasis on options recently added to the code. Among the new options are an energy-dependent direct-capture component for capture cross sections, a crystal-lattice model for Doppler broadening, improvements in the fitting procedure to incorporate more of the experimental uncertainties and covariances, streamlined input, and enhanced ENDF-related capabilities.

INTRODUCTION

The main features of SAMMY [1,2] (or of any code designed for analysis of cross section data) can be sorted into four categories: (1) Calculation of theoretical cross sections. In the resolved-resonance region (RRR), this is usually accomplished via R-matrix theory [3]; in the unresolved-resonance region (URR) various models may be used. (2) Corrections for experimental effects. This category includes any condition (e.g., Doppler broadening) that causes the measured quantity to differ from the quantity whose value is intended to be determined by this experiment. (3) The fitting procedure, the purpose of which is to determine those values for the parameters that provide the best fit of calculated to experimental data. (4) Other features, including input/output and pre- or post-processing functions.

Implementation of these features in SAMMY is described here, with emphasis on recent developments.

THEORETICAL CROSS SECTIONS

In the RRR, the calculation of theoretical cross sections is performed in SAMMY using the Reich-Moore approximation to multilevel multichannel R-matrix theory. For most nuclear data in the RRR, Reich-Moore is generally regarded as the method of choice [4].

Because there may be a need for calculating single-level or multilevel Breit-Wigner cross sections (for example, for comparison with older evaluations), SAMMY also provides this capability. However, use of either of the Breit-Wigner formalisms for new analyses is strongly discouraged, because these approximations can lead to unphysical cross section values.

Occasionally, even the usually-appropriate Reich-Moore approximation is inadequate: When there is level-level interference in capture, for example, then the full (un-approximated) R-matrix is required. Also, for analyses of experiments involving light elements (e.g., $n+{}^6\text{Li}$), the full R-matrix is usually employed. While the full R-matrix has not yet been implemented in SAMMY, experience has shown that it is possible to use the Reich-Moore formalism to calculate the full R-matrix with as much accuracy as desired.

The method for accommodating interference involving capture channels in SAMMY is as follows: give a very small value (e.g., 0.001 meV) for the Reich-Moore capture width, specify a reaction channel with appropriate quantum numbers for capture (that is, use the same quantum numbers as for a fission channel), and provide the actual width for the interfering capture channel in the corresponding location for the reaction channel in the SAMMY parameter file. Note that it is not possible to give a zero value for the Reich-Moore capture width, as this will cause numerical problems in the calculation.

The derivation of R-matrix theory is predicated on the existence of a compound nuclear state; hence a direct reaction is not described by R-matrix theory. In SAMMY, it is now possible to add an energy-dependent direct-capture contribution to the R-matrix component for capture (and therefore also for total) cross section calculations. The direct-capture contribution must be generated externally to SAMMY, for example via direct-semidirect neutron capture calculations such as those performed by Arbanas et al. [5]. Results are input into SAMMY as a numerical function of energy. During the analysis process, the overall normalization of the direct-capture contribution may be varied to determine the absolute magnitude.

In the URR, SAMMY uses Hauser-Feshbach theory with width fluctuations. Froehner's FITACS code [6] is the basis for SAMMY's URR capabilities.

CORRECTIONS FOR EXPERIMENTAL EFFECTS

In the RRR, experimental conditions can cause the measured quantity to be quite different from the theoretical cross sections, and these conditions must be simulated in the analysis code. Examples of this are Doppler broadening (corrections for non-zero temperature of the sample), resolution broadening (e.g., corrections for finite size of the detector system), and background subtraction.

Doppler Broadening

For most experiments, even those involving very heavy nuclides, Doppler broadening can reasonably be described by the free gas model, which is (as the name implies) based on the assumption that the target nuclide behaves as if it were a free gas. Occasionally, however, solid-state effects can be seen in the measurements. To describe these effects, SAMMY now has an option to use a crystal-lattice model (CLM) of Doppler broadening, based on the DOPUSH code of Naberejnev [7] and MacFarlane [8]. Use of SAMMY's CLM is discussed in another paper at this conference [9].

Resolution Broadening

Unlike Doppler broadening, resolution broadening has no single description that applies to all experimental situations. Different resolution functions

are required to describe differences in the burst width and shape, in the detector characteristics, and in the time-channel configurations. Hence SAMMY offers a variety of options for resolution broadening.

The simplest and fastest-running resolution function uses a Gaussian plus exponential tail. (This function is denoted "RSL.") In the initial stages of an analysis, this version may be sufficient even though it is not completely accurate.

More sophisticated resolution functions are formed by modeling the components separately and then convoluting them to give the complete function. Two such "realistic" resolution functions are available in SAMMY: the Oak Ridge resolution function (ORR, developed for use with data from the Oak Ridge Electron Linear Accelerator) and the RPI resolution function (developed initially for use with data from the Rensselaer Polytechnic Institute's Gaertner LINAC).

[About a year ago, a bug was discovered and eradicated in the calculation of the partial derivatives with respect to parameters of the ORR or the RPI resolution function. Treating any of those parameters as fitting parameters during the analysis process will produce better results with future releases of SAMMY, beginning with M7 which will be released in 2005.]

Also available in SAMMY is a user-defined resolution (UDR) function, a numerical function of energy and time. While the UDR has been used successfully, it must always be used with great care: In principal, it is possible to define several numerical functions which SAMMY will then convolute to give the complete resolution function. In practice, the implementation of the convolution procedure in the code is less than optimal. (This limitation will be corrected in the future.)

A straight-line energy-averaging resolution option (denoted DEX) has been implemented in SAMMY, primarily for use in analyses involving charged-particle projectiles.

Combinations of several types of resolution functions can also be used: RSL plus DEX plus one of ORR, RPI, or UDR.

Recent work by F. Gusing [10] has established that extensions of the RPI resolution function will be useful for data taken at the Geel and nTOF facilities. These extensions have been implemented into SAMMY and are currently undergoing testing; a detailed description will be presented elsewhere [11]. The Geel and nTOF resolution functions will be available in the next release of the code.

Others

Angle-averaging is now available in SAMMY for angular-distribution analyses. For analysis of fission or capture yields, SAMMY can provide multiple-scattering corrections. Normalization and energy-dependent background options are possible for analysis of all types of data.

In the URR, energy-dependent normalizations can be assigned to each data set.

FITTING PROCEDURE

SAMMY uses an iterative form of Bayes' Equations (generalized least squares) to find those parameter values that give the best fit of calculated cross sections to experimental data. Uncertainties and correlations on the experimental data are treated accurately and with minimal cost via techniques recently added to the code. (By "minimal cost" is meant minimal computer memory, minimal computation time, and minimal effort on the part of the analyst.) Algebraic manipulation of the matrix components of the data covariance matrix (DCM) has permitted the solution of Bayes' Equations without explicitly generating, storing, or inverting the large DCM; this technique is denoted the "implicit data covariance" (IDC) method. The components of the DCM can be either user-supplied and/or calculated internally by SAMMY.

Any parameter that SAMMY is capable of varying (i.e., almost any parameter related to either theory or experimental conditions, as discussed in the two previous sections) may now be treated as a "propagated uncertainty parameter" (PUP). The previously-determined uncertainty on a PUP will be propagated through the analysis process, but the value of the PUP will not be changed.

Both PUPs and the IDC method are described in more detail in another paper at this conference [12].

All covariance matrices occurring in SAMMY are now automatically tested for positive definiteness, and any failures are reported to the user.

In addition to calculating and reporting the best-fit parameter values at the end of a run, SAMMY also reports the associated parameter covariance matrix. However, with all previous public releases of the SAMMY code, when both the resonance energy and the neutron width are flagged (varied), the reported

parameter covariance matrix will not be completely correct. A mistake has been found, related to the change-of-variable from reduced-width amplitude γ to partial width $\Gamma = 2P\gamma^2$; the former is used internally in SAMMY, while the latter is reported in the output files. When the original transformation of the parameter covariance matrix was implemented, the resonance-energy-dependence of the penetrability P was overlooked. This oversight has been corrected for the next release of the code.

Fortunately, consequences of this mistake should not be significant: until recently, parameter covariance information has not been reported, either in the open literature or in the ENDF files. This is changing, as described in other papers at this conference [13, 14]. (It was, in fact, in the course of comparing SAMMY results with results from Chiba's ERRORJ code [14] that this mistake was uncovered.)

OTHER FEATURES

As more options are created for SAMMY, the input has necessarily become more complicated. Efforts are continuing to provide simpler formats with fewer possibilities for human error. Among other changes, keyword-based input is implemented whenever possible.

Quantum Numbers

A streamlined format has been developed for input of spin-group information for the RRR. In this format, the particle-pair information is provided separately from the channel quantum numbers to avoid unnecessary repetition of the same information. To further simplify the SAMMY user's task, an auxiliary code has been created to help prepare the quantum-number input for SAMMY. This code, named SAMQUA [15], was coauthored by colleagues from the French Atomic Energy Commission at Cadarache; recent enhancements to SAMQUA are presented in a separate paper at this conference [16].

ENDF Formats

Two new Evaluated Nuclear Data File (ENDF) formats, provisionally approved by the Cross Section Evaluation Working Group during the 2003 meeting, now permit translation of any SAMMY evaluation into formats suitable for inclusion in ENDF.

The “R-matrix limited” format is used to report R-matrix resonance parameter values in the case where there are several entrance channels, more than two exit channels, one or more threshold reactions, and/or charged-particle channels. The code SAMRML (a modified version of relevant portions of the SAMMY code) can be used to read resonance parameters from this format and calculate cross sections and partial derivatives. SAMRML has been made available to processor-code developers for incorporation into their codes or for testing purposes.

The “compact covariance matrix” format can be used for storing resonance-parameter covariance information in an approximate fashion for those cases where the size of the matrix prohibits storage of the complete matrix.

SAMMY can read and write resonance parameter and covariance information in both of these new formats, as well as in many of the earlier ENDF formats. See the SAMMY manual [1] for details.

SUMMARY AND FUTURE PLANS

In this paper, a description of the main features of the SAMMY code has been provided. Enhancements to the code subsequent to the previous Nuclear Data Conference are announced.

In addition to further testing on the Geel and nTOF resolution functions as described earlier, other enhancements to SAMMY are planned: The CLM for Doppler broadening will be tested and possibly extended. Multiple-scattering corrections will be studied further to see if refinements can be made to the double-plus scattering contribution. Capability for truly simultaneous analysis of several data sets will be added. In the URR, calculations of integral quantities will be implemented, as will the capability for including more than one nuclide in the sample. Creation of a workable and portable graphical user interface will be considered.

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